

## **Carbon Nanotubes - Miracle of Materials Science?**

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Imagine a single molecule that is 50,000 times thinner than a human hair and 100 times stronger than steel. Such a molecule is invisible to the naked eye, yet could revolutionize materials technology. Scientists have mastered the synthesis and characterization of components on the microscopic scale; however, the discovery of carbon molecules called nanotubes has sparked new interest in materials on the nanoscale (100 nm or less). Carbon nanotubes are constructed of a graphene sheet rolled into a tube with fullerene caps on the ends. These single-walled elongated fullerene molecules contain millions of carbon atoms, each atom occupying an assigned place to form defect-free hollow structures just a few atoms in circumference. A nanotube's length is many thousands of times longer than its diameter and possesses exceptional mechanical, electrical, and thermal properties.

With tensile strengths at least 10 times stronger and less than half the weight of conventional carbon fiber, electrical conductivity as high as copper and thermal conductivity as high as diamond, carbon nanotubes<sup>†</sup> can serve multifunctional roles. Properties can be tailored through processing to fit a multitude of aerospace, biomedical, and industrial applications. The range of applications for such properties is endless – from chemical sensors and high strength composites to tiny networks transporting telemetry in a biomimetic fashion. Historically, biological systems have operated on atomic scale principles; now engineers will be able to explore this amazing nanoworld in the same intricate fashion. Welcome to the world of carbon nanotechnology!

### **Mechanical Properties**

Absence of defects in individual nanotubes enhances their mechanical properties and potential for use as structural reinforcement. Rigorous bonds are formed from covalently-linked carbon atoms having three nearest neighbors. Tube ends are sealed with no dangling chemical bonds to weaken the arrangement. The lightweight structure is assembled as an ideal carbon fiber that has the strongest bonds found in nature. Cohesive strength between carbon atoms and high elasticity compared to that of graphite fibers make nanotubes highly resistant to failure under tension.

Nanotubes are known to have a tensile strength of 50-200 GPa, which is at least an order of magnitude higher than conventional graphite fibers. Additionally, predictions of high elasticity and bending stiffness are supported by thermal vibration amplitude

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<sup>†</sup> Depending on the processing method nanotubes may have multiple walls with concentric cylinders around the inner tube. Multi-walled tubes contain imperfections and exhibit properties comparable to conventional carbon fibers, therefore single-walled tubes are of primary interest for materials development. For clarity the single-walled variety will be referred to as nanotubes.

**ABSTRACT OR SUPPORTING INFORMATION**

Article to be sent to Advanced Materials and Processes, journal of ASM International, as attached. This is a news-type technical journal for a large organization of scientists, engineers, salesmen, and managers. The article is quite general, meant to be an introduction to the properties of nanotubes. This is a materials science organization, therefore the article is geared toward using nanotubes for materials uses. Pictures have not been included in this version.

measurements of Young's modulus of over 1 Tera Pa. Nanotubes are expected to break at very high strain (5-20%), and in dynamics simulations they behave like "superstrings": narrowing down to single carbon chains upon application of tension. Flexibility and resiliency in the direction normal to the tube surface are evidenced by the triangular lattice of nanotubes that bend through the image plane of a microscope as shown in Figure 2b. Nanotubes also exhibit resistance to distortion from torsional forces, and in many cases the original cross-section of the nanotubes is restored when the load is released. Unlike graphite fibers that fracture easily under compression, nanotubes form kink-like ridges under compression that relax elastically after loading. Such properties are directly applicable to a variety of engineering structural applications including high strength composites and textile weaves.

High modulus and high elastic strain of nanotubes qualifies them as a potential reinforcement phase in composite materials. Microcracks in continuous solids act as stress concentrators, but the failure of one fiber in a composite of loosely-coupled nanotubes would result in very little overloading of adjacent tubes; crack growth would be suppressed. Loads are effectively transferred to the nanotubes, resulting in a composite modulus that is similar to that of an isotropic short fiber composite containing fibers of exceptional modulus and tensile strength.

The high surface area of nanotubes (compared to graphite fibers) creates a large interfacial region that can have different properties from the bulk matrix. Although interfaces have always been important in composites, the interfacial regions are now so numerous that they dominate the behavior of the bulk material. Evidence of increased interaction between matrix and fiber is manifest in the fracture surface micrographs shown in Figure 3 of nanotubes dispersed in a thermosetting polymer. Dispersion of nanotubes on the microscopic scale is apparent and some load transfer occurs between the matrix and reinforcement. One method for increasing this load transfer is to attach molecules to the ends or sides of nanotubes for better bonding. Functionalization at the molecular level brings a new level of design to composite materials beyond common methods for increasing interfacial adhesion. It is unknown at this time how the addition of certain functional groups affects the mechanical strength of the tubes. Due to known extraordinary mechanical properties of nanotubes, development of high strength composites remains a worthy but difficult goal.

## **Electrical Properties**

The range of applications of nanotubes extends beyond reinforcement in material systems due to their unique structure-dependent electrical properties. Depending on how the hexagonal chains are oriented relative to the tube axis (chirality), they may act as metals or semiconductors. A "rollup" vector (n,m) specifies the oriented tube diameter and describes the number of steps in directions a and b as shown in Figure 4. The chirality of the tubes is also known to affect their mechanical properties, an important point when researching composite materials.

Assembly of nanotubes in this manner results in a hybridization of electron bonds that differs from both diamond and graphite. Three of four valence electrons around carbon atoms form in-plane bonds, leaving free electrons to travel in one dimension along the tube rather than two dimensions that are available in the graphene plane. A significant increase in carrier electron density is expected in a parallel bundle of nanotubes, resulting in conductivity comparable to a good metal. Recent measurements of the conductance in metallic nanotubes shows a stepwise conductance with increasing voltage, which indicates a quantum-level behavior and potential for nanotubes to be used as molecular wires in devices that rival existing transistors, field emitters, and electrostatic discharge materials. Progress towards molecular electronics is evidenced by the recent demonstration of diodes and field effect transistors based on single wall carbon nanotubes. It is also noted that doping with other elements like potassium or bromine can control the electrical characteristics of nanotubes. The application of nanotubes for flat panel displays and commercial lighting may prove possible with the recent demonstration of its field emitting properties under ambient conditions.

### **Thermal Properties**

The structure of nanotubes has a profound influence on heat transport properties in both the parallel and transverse dimensions. Since nanotubes are constructed of a single rolled graphene sheet, the thermal conductivity along the sheet has been measured to be comparable to that of diamond (the highest thermal conductor). These one-dimensional tubes have very high aspect ratios (length to diameter), and most of the heat is expected to be transported along their length. Therefore, a material of highly anisotropic thermal conductivity could be synthesized using aligned tubes.

While heat transport in the parallel dimension is expected to rival the best conductor, the rate of heat transfer in the perpendicular direction is much lower. The transverse dimension of nanotubes is an order of magnitude larger than the most probable wavelengths of lattice vibrations (phonons) in dielectrics from room temperature to 1500°C. Similarities between the transverse dimension and phonon wavelength should make dispersed nanotubes effective in forming interfaces that scatter phonons and reduce thermal conductivity.

### **Nanotube Research Status**

Nanotube research is limited by the scarcity and expense of nanotubes due to the lack of a bulk production method. Arc and laser production techniques produce only enough materials for small-scale research. If a method can be found to make large quantities, then research will accelerate and become a major field in materials science and other areas of science and engineering. Current research in nanotube production focuses on gas-phase processes including chemical vapor deposition. Recent results are encouraging, but the breakthrough to finding an industrial-scale process remains elusive.

United States, European, and Asian government initiatives show international commitment to nanotechnology. The U.S. Government's involvement has emerged from an Interagency Workgroup on Nanoscience, Engineering, and Technology, led by the National Science Foundation. NASA has been interested in nanotubes for several years and maintains a close collaboration with a number of businesses and universities, including Richard Smalley's research group at Rice University. Applications in such areas as materials science, energy storage, nanoelectronics, and biomedicine are current areas of interest. At the Lyndon B. Johnson Space Center in Houston, Texas, interest focuses on developing high strength composite materials for use in next-generation spacecraft. Because of the high weight penalty for interplanetary missions, NASA is looking for revolutionary technologies such as inflatable spacecraft, spacesuits, and hypervelocity impact shielding. As nanotube availability increases, it will be up to researchers to make this promise into reality. NASA realizes that the biggest breakthrough in enabling visits to other planets could evolve from technology breakthroughs at the molecular and atomic levels. Manipulation of items on the nanoscale allows us to reach toward the fantastic engineering found in biological mechanisms, but we may have a long way to go.

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### **Captions:**

Fig. 1 - Arc furnace production method; nanotube formation visible around cathode deposit (right).

Fig. 2 – (a) Scanning electron microscope (SEM) image of nanotube bundles, as produced by the laser ablation system; (b) Transmission electron micrograph (TEM) cross-sectional view of nanotube "rope" bending through image plane.

Fig. 3 – (a) SEM image of nanotube composite, showing dispersion of tubes; (b) TEM photograph shows wetting between fiber bundles and epoxy matrix.

Fig. 4 - (a) Nanotubes ends are sealed with spherical fullerene molecules ; (b) A rollup vector (n,m) specifies tube width and number of steps across hexagonal chains.